

# Shift of BEC Temperature of Homogenous Weakly Interacting Bose Gas\*

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(Dated: September 2003)

We report on the computation of the shift of the Bose-Einstein condensation temperature for a homogenous weakly interacting Bose gas in leading order in the diluteness parameter  $an^{1/3}$ , where  $a$  is the scattering length and  $n$  is the particle density. The perturbative series, which is afflicted by infrared divergences, is resummed by means of variational perturbation theory. Using coefficients through seven loops, we arrive at  $\Delta T_c/T_c = 1.27 \pm 0.11 an^{1/3}$ , which compares favorably with recent Monte-Carlo data.

PACS numbers: 03.75.Hh, 05.30.Jp, 12.38.Cy

## I. INTRODUCTION

The Bose-Einstein condensation (BEC) temperature  $T_c$  of an ideal gas of spin-0 Bosons is given by

$$T_0 = \frac{2\pi}{m} \left[ \frac{n}{\zeta(3/2)} \right]^{2/3}, \quad (1)$$

where  $m$  is the mass of the bosons,  $n$  their number density and we work throughout in units where  $k_B = \hbar = 1$ . Infrared (IR) divergences prevent the perturbative evaluation of the shift of the BEC temperature due to a small repulsive interaction, parameterized by the corresponding  $s$ -wave scattering length  $a$ . Physically, these IR divergences correspond to critical fluctuations that change the universality class from Gaussian to that of a three-dimensional scalar  $O(2)$ -symmetric field theory.

Although it is clear that  $T_c$  changes by a small amount if the dimensionless diluteness parameter  $an^{1/3}$  is small (for small momenta,  $a$  is the only relevant parameter of the two-body interaction potential), it was for a long time unclear, what the leading power in terms of this parameter or the coefficient in front of it would be. Many attempts on the problem have provided different powers and coefficients [1–24]. Recently, however, it has been shown that the leading and next-to-leading behavior is given by [7, 8, 15]

$$\frac{\Delta T_c}{T_0} = c_1 an^{1/3} + [c'_2 \ln(an^{1/3}) + c''_2](an^{1/3})^2 + \dots \quad (2)$$

In the work presented here, we determine  $c_1$  numerically (while  $c'_2$  is known exactly,  $c''_2$  may be determined by a non-perturbative calculation analogous to the one presented here for determining  $c_1$ ; for the exact value of  $c'_2$

and a MC estimate of  $c'_2$ , see Ref. [16]). Results for  $c_1$  in the literature range from  $-0.93$  [9] to  $4.7$  [2], see Refs. [14, 17] and the review [25], also Fig. 1 below. In [7] it was shown that  $c_1$  is exclusively generated by infrared fluctuations and that consequently three-dimensional field theory is sufficient for the determination of  $c_1$ . It appears that the most reliable results for  $c_1$  before our work have been obtained by Monte-Carlo (MC) simulations in three-dimensional field theory [13, 14].

Here we expand  $\Delta T_c$  in a perturbative series, which is subsequently resummed to obtain the physical non-perturbative limit. While simple schemes such as Padé approximants may slowly converge towards the correct value, our scheme of choice is Kleinert's field theoretic variational perturbation theory (VPT, see [26–28] and Chapters 5 and 19 of the textbooks [29] and [30], respectively; improving perturbation theory (PT) by a variational principle goes back at least to [31]), which has proven very useful for the investigation of critical phenomena.

## II. FIELD THEORY

The thermodynamic equilibrium properties of a homogenous gas of spin-0 Bosons may be described in the grand canonical ensemble with the help of a non-relativistic  $(3+1)$ -dimensional field theory in imaginary time  $\tau$ , given by the Euclidean action

$$S_{3+1} = \int_0^\beta d\tau \int d^3x \left[ \psi^* \left( \frac{\partial}{\partial \tau} - \frac{1}{2m} \nabla^2 - \mu \right) \psi + \frac{2\pi a}{m} (\psi^* \psi)^2 \right], \quad (3)$$

where  $\mu$  is the chemical potential. This assumes that the momenta of the particles are small enough so that their interaction potential is well described by just one parameter, the  $s$ -wave scattering length  $a$ . It also assumes that three- and more particle interactions are rare, i.e. that the gas is dilute. It turns out that the leading perturbative contribution to  $\Delta T_c$  is  $\propto a^2$ . In consequence,

\*Talk presented at the 12th International Laser Physics Workshop, LPHYS'03 (Hamburg, Germany, August 25-29, 2003).

the leading contribution to  $\Delta T_c$  arises exclusively from terms that are infrared divergent in the framework of PT. This is why, for the determination of  $c_1$ , we can set all Matsubara frequencies to zero or, equivalently, work with a three-dimensional field theory [7]. Denoting the zero-Matsubara modes by  $\psi_0$ , we define the fields and parameters of this theory by  $\psi_0 = \sqrt{mT}(\phi_1 + i\phi_2)$ ,  $r_{\text{bare}} = -2m\mu$ ,  $u = 48\pi amT$ , and obtain the three-dimensional Euclidean action

$$S_3 = \int d^3x \left[ \frac{1}{2} |\nabla \phi|^2 + \frac{r_{\text{bare}}}{2} \phi^2 + \frac{u}{24} (\phi^2)^2 \right]. \quad (4)$$

For the determination of quantities that are not governed by the leading IR divergences, one may still use a three-dimensional field theory which, however, is obtained by a more complicated matching procedure, which introduces corrections to the above relations of the parameters of the (3+1)-dimensional and the three-dimensional theory and also necessitates the inclusion of more interaction terms. This matching is described in detail in [16].

From the ideal-gas result (1) one obtains, in leading order, the relation [7]

$$\frac{\Delta T_c}{T_0} = -\frac{2}{3} \frac{\Delta n}{n}, \quad (5)$$

where  $\Delta T_c$  is the shift of the condensation temperature for fixed  $n$  and  $\Delta n$  is the shift of the critical particle density for fixed condensation temperature. In our field-theoretic setup,  $\Delta n$  is given by

$$\Delta n = \Delta \langle \psi^* \psi \rangle = mT \Delta \langle \phi^2 \rangle. \quad (6)$$

Combining (1), (2), (5) and (6),  $c_1$  is given by

$$c_1 = \alpha \left. \frac{\Delta \langle \phi^2 \rangle}{Nu} \right|_{\text{crit.}} \quad (7)$$

with  $\alpha = -256\pi^3/[\zeta(3/2)]^{4/3} \approx -2206.19$  and the remaining task is to compute the critical limit of

$$\frac{\Delta \langle \phi^2 \rangle}{Nu} = \frac{1}{u} \int \frac{d^3p}{(2\pi)^3} [G(p) - G_0(p)] \equiv \frac{1}{u} \left[ \text{diagram} - \text{diagram} \right], \quad (8)$$

where  $G$  and  $G_0$  are the interacting and the free propagator, respectively. In (7) and (8) we have conveniently generalized the model (4) to an  $O(N)$  field theory, where  $\phi = (\phi_1, \dots, \phi_N)$ ,  $\phi^2 \equiv \phi_a \phi_a$ . This allows to make contact with the exactly known large- $N$  result for  $c_1$  [8] and with the MC results for  $N = 1$  and  $N = 4$  [32].

The theory (4) is superrenormalizable. A convenient and popular renormalization scheme is given by defining a renormalized parameter  $r = r_{\text{bare}} - \Sigma(0)$ , where  $\Sigma(p)$  is the self-energy. Now all Feynman diagrams can be computed without regularization. The critical limit is obtained by letting  $r \rightarrow 0$ , as can be seen from the structure of the full propagator, which reads now  $G(p) = 1/\{p^2 + r - [\Sigma(p) - \Sigma(0)]\}$ . For the free propagator follows  $G_0(p) = 1/(p^2 + r)$  [20].

In a scheme used in [12, 18, 19, 22, 33], the free propagator is taken always critical,  $G_0(p) = 1/p^2$ . This generates an unnatural non-zero one-loop contribution to  $\Delta \langle \phi^2 \rangle$ , even in the absence of interactions. Although this contribution vanishes as  $r \rightarrow 0$ , it strongly influences resummation and is responsible for the small value of  $c_1 = 0.92 \pm 0.13$  [34] in Ref. [22].

### III. PERTURBATIVE SERIES FOR $c_1$

In PT,  $\Delta \langle \phi^2 \rangle / Nu$  may be written as a power series in  $u_r \equiv Nu/4\pi r^{1/2}$ . Defining a function  $c_1(u_r)$  with  $c_1 = \lim_{u_r \rightarrow \infty} c_1(u_r)$ , we have

$$c_1(u_r) = \alpha \sum_{l=1}^{\infty} a_l u_r^{l-2}. \quad (9)$$

The inclusion of  $N$  in the definition of  $u_r$  is motivated by the fact that then the  $a_l$  remain finite even in the limit  $N \rightarrow \infty$ , facilitating the comparison with the exactly known large- $N$  result [8]. The successful application of VPT to the large- $N$  limit has been demonstrated in [23].

The perturbative series can be represented by Feynman diagrams and then becomes a loop expansion. The subtraction of the zero-momentum part of the self-energy in the full propagator has to be performed recursively for all subdiagrams. We denote this procedure by an operator  $\mathcal{R}$  [23, 24]. The first non-zero perturbative coefficient arises at the three-loop level, since the lowest momentum-dependent self-energy contribution has two loops. The perturbative coefficient at  $L$  loops is given by

$$a_L u_r^{L-2} = \frac{1}{Nu} \sum_{k=1}^{n_L} \mathcal{R} D_{L-k}, \quad (10)$$

where  $n_L$  is the number of contributing diagrams in  $L$ -loop order and  $D_{L-k}$  is the  $k$ -th  $L$ -loop diagram. There are  $n_L = 0, 0, 1, 1, 5, 12, 56$  diagrams at one- through seven-loop order (see [35] for a convenient way of constructing all necessary diagrams together with their weights) and the expansion for  $c_1(u_r)$  starts out as

$$c_1(u_r) = \frac{\alpha}{Nu} \left[ \mathcal{R} \left( \text{diagram} \right) + \mathcal{R} \left( \text{diagram} \right) + \mathcal{R} \left( \text{diagram} \right) + \mathcal{R} \left( \text{diagram} \right) + \mathcal{R} \left( \text{diagram} \right) + \mathcal{R} \left( \text{diagram} \right) + \mathcal{R} \left( \text{diagram} \right) + \dots \right]. \quad (11)$$

E.g., the coefficient  $a_3$  is given by

$$a_3 u_r = \frac{1}{Nu} \mathcal{R} \left( \text{diagram} \right)$$

$$\begin{aligned}
&= \frac{(N+2)u}{18} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \frac{1}{(k^2+r)^2} \\
&\quad \times \left[ \frac{1}{(k+p)^2+r} - \frac{1}{p^2+r} \right] \frac{1}{[(p+q)^2+r](q^2+r)} \\
&= -\frac{(1+\frac{2}{N})\ln\frac{4}{3}}{576\pi^2} u_r. \tag{12}
\end{aligned}$$

The results for diagrams through six loops in the renormalization scheme employed here can be found in [36]. The seven-loop diagrams have been computed in 1991 and used for the determination of critical exponents for  $N = 0, 1, 2, 3$  in [37]. They were provided to the author by B. Nickel [38] and may be found in [24]. The resulting perturbative coefficients for  $N = 2$  are  $a_3 = -1.01209 \times 10^{-4}$ ,  $a_4 = 2.99626 \times 10^{-5}$ ,  $a_5 = -1.19872 \times 10^{-5}$ ,  $a_6 = 5.85519 \times 10^{-6}$ ,  $a_7 = -3.30467 \times 10^{-6}$ .

#### IV. RESUMMATION AND RESULTS

For obtaining the  $u_r \rightarrow \infty$  limit of  $c_1(u_r)$ , the series (9) needs to be resummed. For critical fluctuations phenomena, VPT is an appropriate tool, since it is designed to accommodate the large- $u_r$  behavior of physical quantities in the critical limit, given in our case by

$$c_1(u_r) = \alpha \sum_{m=0}^{\infty} f_m u_r^{-m\omega'} \tag{13}$$

with an irrational exponent  $\omega'$ . The leading class of corrections of a physical quantity that remains finite in the critical limit are integer powers of  $t^{\omega\nu}$  [30, 39, 40], where  $t \equiv (T - T_c)/T_c$ ,  $\nu$  is the critical exponent of the correlation length and  $\omega = \beta'(g^*)$  in a renormalization group approach. In our renormalization scheme, the propagator obeys  $G(p=0) = 1/r \propto t^{-\gamma}$ . Using the universal scaling relation  $\gamma = \nu(2 - \eta)$ , where  $\eta$  is the anomalous dimension of the critical propagator, i.e.  $G(r=0) \propto 1/p^{2-\eta}$  in the small- $p$  limit, we see that we have to set

$$\omega' = \frac{2\omega}{2-\eta} \tag{14}$$

in (13).

The ansatz (13) does not account for so-called confluent singularities which cause the true large- $u_r$  expansion to also contain other negative powers of  $u_r$ , which are subleading at least compared to  $u_r^{-\omega'}$ . We can expect methods that can accommodate the leading behavior in (13) correctly to converge faster to the true result than methods having the wrong leading behavior such as e.g. Padé approximants or the linear  $\delta$  expansion (LDE), the latter being used extensively for the current problem [12, 18–21]. On the other hand, convergence will be slowed by the fact that we do not make an ansatz reflecting the full power structure in  $u_r$ , but the expansion (13) will try to mimic the neglected subleading powers.

The alternating signs of the  $a_L$  suggest that the perturbative series for  $c_1(u_r)$  is Borel summable. In the context

of critical phenomena, such series have been successfully resummed using Kleinert's VPT. Accurate critical exponents [27, 28, 30] and amplitude ratios [41] have been obtained. For a truncated partial sum  $\sum_{l=1}^L a_l u_r^{l-2}$  of (9), the method requires replacing

$$u_r^{l-2} \rightarrow (t\hat{u})^{l-2} \left\{ 1 + t \left[ \left( \frac{\hat{u}}{u_r} \right)^{\omega'} - 1 \right] \right\}^{-(l-2)/\omega'} \tag{15}$$

(note that this is an identity for  $t = 1$ ), reexpanding the resulting expression in  $t$  through  $t^{L-2}$ , setting  $t = 1$  and then optimizing in  $\hat{u}$ , where optimizing is done in accordance with the principle of minimal sensitivity [42] and in practice means finding appropriate stationary or turning points. That is, we replace

$$u_r^{l-2} \rightarrow \hat{u}^{l-2} \sum_{k=0}^{L-l} \binom{-(l-2)/\omega'}{k} \left[ \left( \frac{\hat{u}}{u_r} \right)^{\omega'} - 1 \right]^k \tag{16}$$

and optimize the resulting expression in  $\hat{u}$ . For  $u_r \rightarrow \infty$ , we obtain the  $L$ -loop approximation of  $f_0$ ,

$$f_0^{(L)} = \text{opt}_{\hat{u}} \left[ \sum_{l=1}^L a_l \hat{u}^{l-2} \sum_{k=0}^{L-l} \binom{-(l-2)/\omega'}{k} (-1)^k \right]. \tag{17}$$

Results are only available starting at four loops, since two non-zero perturbative coefficients are necessary for VPT to work. E.g., in four-loop order the optimization yields

$$f_0^{(4)} \approx \text{opt}_{\hat{u}} \left[ a_3 \left( 1 + \frac{1}{\omega'} \right) \hat{u} + a_4 \hat{u}^2 \right] = -\frac{a_3^2 \left( 1 + \frac{1}{\omega'} \right)^2}{4a_4} \tag{18}$$

as the best attempt at determining  $f_0$  and thus  $c_1 = \alpha f_0$ .

For  $N = 2$ , we have  $\omega = 0.79 \pm 0.01$ ,  $\eta = 0.037 \pm 0.003$  (see, e.g., [30]) and thus, using (14),  $\omega' = 0.805 \pm 0.011$ . The four- through seven-loop results are  $c_1 = 0.948, 1.062, 1.126, 1.161$ .

$\omega'$  may also be determined self-consistently [27, 29, 30]. Assuming a behavior of  $c_1(u_r)$  as in (13), the quantity  $d \ln c_1(u_r)/d \ln u_r$  has an expansion of the same type with the same  $\omega'$  as  $c_1(u_r)$ , but with a vanishing large- $u_r$  limit (i.e. its large- $u_r$  expansion starts out with  $f_0 = 0$ ).  $\omega'$  is tuned such that the value VPT gives for  $d \ln c_1(u_r)/d \ln u_r$  is zero in a given loop order. This  $\omega'$  is then used as an input for the determination of the approximation of  $c_1(u_r)$  at the same loop order. The five- through seven-loop results are  $c_1 = 1.399, 1.383, 1.376$ .

From the fact that the fixed- $\omega'$  results monotonically rise with the loop order, while the results with self-consistent  $\omega'$  fall, we estimate that the true value lies inbetween and conclude from the resummed results through seven loops that

$$c_1 = 1.27 \pm 0.11. \tag{19}$$

Our treatment for  $N = 2$  may easily be repeated for arbitrary  $N$ . E.g., for  $N = 1$  one obtains

$$c_1 = 1.07 \pm 0.10, \tag{20}$$

while for  $N = 4$ , the result is

$$c_1 = 1.54 \pm 0.11. \quad (21)$$

## V. DISCUSSION

Many different results have been obtained for  $c_1$ ; see [24] and corresponding references therein for criticisms of most of them. A comparison of our results through seven loops with most other results found in the literature is given in Fig. 1. Our result (19) is in agreement with the

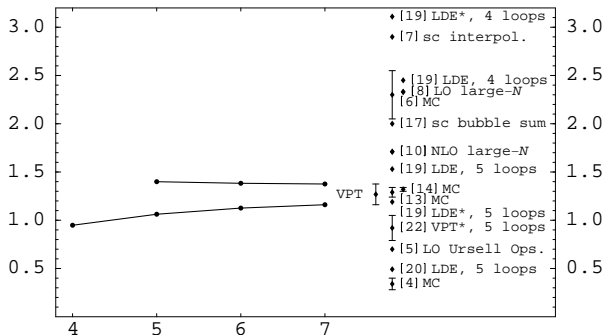


FIG. 1: Comparison of  $c_1$  from VPT as a function of the number of loops  $L$  for  $N = 2$  with most results from other sources. Upper dots: self-consistent (sc)  $\omega'$ . Lower dots:  $\omega' = 0.805$ . LDE\* indicates use of LDE with a resummation method for accelerated convergence. The label VPT\* indicates the inclusion of a non-zero one-loop term in Ref. [22], which is absent in the present treatment, labeled by VPT.

apparently most reliable other sources available, namely the MC results from the three-dimensional theory:  $c_1 = 1.29 \pm 0.05$  by Kashurnikov, Prokof'ev and Svistunov [13] and  $c_1 = 1.32 \pm 0.02$  by Arnold and Moore [14].

MC results for  $N = 1$  and  $N = 4$  are also available. X. Sun has computed  $\Delta\langle\phi^2\rangle_{\text{crit.}}/u$  for these cases [32]

which translate to  $c_1 = 1.09 \pm 0.09$  for  $N = 1$  and  $c_1 = 1.59 \pm 0.10$  for  $N = 4$ . Our values (20) and (21) agree well with these results. This provides additional confidence that in fact both MC and our VPT results are trustworthy estimates for  $c_1$ .

We would like to emphasize that the coefficient  $c_1$  is of physical relevance not only for the case of a strictly homogeneous gas, but also for a trap that is sufficiently wide to allow for critical fluctuations [10, 43]. If expressed as a function of the total number of particles  $N_p$ , the leading effect on the shift of the condensation temperature is obtained from mean field theory and only in second order the influence of critical fluctuations can be felt [43, 44]. In contrast, if expressed in terms of the central density  $n$  of particles, the leading effect is determined by critical fluctuations as we have seen here. It would therefore be desirable to know not only the total number of particles  $N_p$  (as in a recent experiment [45]) but also the central density of particles in experiments that measure the condensation temperature. In this context we would also like to stress that it is no contradiction that the sign of the change of  $T_c$  is different in both cases, since different physical quantities  $N_p$  and  $n$  are kept fixed, respectively. Let us turn this around: For a given condensation temperature, a small repulsive interaction causes the corresponding central density in a wide trap to be lowered and the total number of particles to be raised compared to the ideal gas case.

## Acknowledgments

The author is extremely grateful to B. Nickel for providing the results of his seven-loop calculations and thus facilitating the extension of the VPT treatment through seven loops. He thanks H. Kleinert, P. Arnold and E. Braaten for valuable input. Helpful communications with J. Andersen, M. Holzmann, F. Laloë, D. Murray, M. Pinto and R. Ramos are also acknowledged.

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